Site Selectivity and Bonding in the β Phase Aluminides: Studies of RuAl, PdAl, and Pd and Ru Dopants in NiAl

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Introduction: Ternary dopant additions to intermetallic hosts can have important effects on the host alloy mechanical properties. We have previously carried out systematic studies of site selectivity and induced local order of such metallic dopants in transition metal (TM) aluminides[1,2]. In the present investigation, we have extended these studies to the case of Ru and Pd ternary dopants in NiAl, and studied local bonding by measuring the temperature dependence of the mean squared relative displacement (MSRD).

Methods and Materials: We prepared stoichiometric β phase RuAl, and Pd and Ru doped NiAl samples. Temperature dependent Ru and Pd fluorescence XAFS was obtained at the X-11 line of the NSLS using Si (111) crystals and a Displex refrigerator. The glancing emergent angle (GEA) mode was used for the RuAl [3] to avoid the distortions that result when fluorescence XAFS is obtained on concentrated samples. We performed further analysis on previously obtained MSRD data for NiAl, CoAl, and FeAl[4] and a new theoretical calculation was performed for the elastic moduli of β phase PdAl by M. Mehl, of the Center for Computational Science, NRL, as part of this project[5].

Results: We find that for both TM rich and poor compositions, the Ru or Pd dopant in NiAl goes to the Ni sublattice. This is in agreement with our previous model relating matrix cohesive energy to dopant site preference[5,1]. That is to say, the cohesive energies of PdAl and RuAl exceed those of NiAl, and therefore, by our model, the Pd or Ru dopants in a NiAl matrix will go to the TM sublattice since these elements bond more strongly to Al in the β phase system than does Ni. We find, from our MSRD results, evidence for a large local shear resistance for Ru dopants in NiAl relative to Pd dopants in NiAl. Finally, from our MSRD results for stoichiometric alloys and literature results for MSRD systematics in monatomic cubic TM materials, we show a linear relationship between bulk shear modulus and the temperature dependence of the MSRD in the linear region of the MSRD versus temperature plot.

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